

The 5th Annual
University of Waterloo
Symposium
on
Chemical Physics

November 3-5, 1989

Acknowledgements

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Waterloo Symposium on Chemical Physics

November 3-5, 1989

at the University of Waterloo

REGISTRATION begins at 7 p.m., Davis Centre Rm. 1301

SESSION I: Friday, November 3, 1989

Davis Centre 1302

Chairman: J.J. Sloan

- 8:00 - 8:40 P. Corkum (NRC, Ottawa)
Femtosecond Lasers for Chemical Physics.
- 8:40 - 9:00 J.M. Dawes, G. Leach, D. Demmer and S.C. Wallace (University of Toronto)
Excited State Proton Transfer in Jet-Cooled 3-Hydroxyflavone and its Hydrogen Bonded Complexes.
- 9:00 - 9:20 T.E. Gough (University of Victoria)
When Is A Cluster Not A Cluster?
- 9:20 - 9:40 W.R. Peifer, M. Todd Coolbaugh and J.F. Garvey (SUNY at Buffalo)
Observation of "Magic Numbers" in the Population Distributions of the $(\text{NH}_3)_{n-1}\text{NH}_2^+$ and $(\text{NH}_3)_n\text{H}_2^+$ Cluster Ions.

SESSION II: Saturday, November 4, 1989 A.M.

Davis Centre 1302

Chairman: K.T. Leung

- 9:00 - 9:40 A.P. Hitchcock (McMaster University).
Inner-Shell Excitation Spectroscopy of Molecules.
- 9:40 - 10:00 N. Moazzen-Ahmadi, A.R.W. McKellar and T. Amano (NRC, Ottawa)
High Resolution Infrared Laser Spectroscopy of the Linear Carbon Chain C_5 .
- 10:00 - 10:20 C. Douketis and J.P. Reilly (Indiana University)
A New Ro-Vibronic Band of Hydroperoxy Free Radical Near 7600Å.
- 10:20 - 10:40 **Coffee Break**
- 10:40 - 11:20 S. Mukamel (University of Rochester)
Solvation Dynamics in Electron Transfer and Nonlinear Optical Susceptibilities: A Unified Description.
- 11:20 - 11:40 H.R. Mayne (University of New Hampshire)
The Effect of Reagent Rotation on Chemical Reactivity.
- 11:40 - 12:00 E.E. Aubanel and D.M. Wardlaw (Queen's University)
Angular Momentum Dependence of Variational Transition States.
- 12:10 - 1:45 **Lunch**

*Chemistry 2-361
Davis Centre 1301*

SESSION III: Saturday, November 4, 1989 P.M.

~~Optometry 347~~
Davis Centre 1302

Chairman: R.J. Le Roy

- 2:00 - 3:00 J.P. Toennies (Max-Planck Institut für Strömungsforschung, Göttingen)
Hot Molecules and Cold Clusters
- 3:00 - 3:20 C.E.D. Chidsey (AT&T Bell Labs), G.-Y. Liu, N. Camillone III and G. Scoles,
(Princeton University)
Law and Order at the Surface of Organic Solids.
- 3:20 - 3:40 T.H. Ellis (Université de Montreal).
The Interaction of Water with Pd(110).
- 3:40 - 4:00 K.G. Soga, H. Haranczyk, R.J. Rumm and M.M. Pintar (University of Waterloo).
Deposition of Water on Silica Glass.

SESSION IV: Saturday, November 4, 1989 P.M.

University Club -UC

POSTER SESSION

- 1) M.A. Kmetc, J.C. Shelley and R.J. Le Roy (University of Waterloo).
Spontaneous Isomerizations and Dynamical Propensities of Some $SF_6-(Ar)_n$ Clusters.
- 2) S.P. Sapers and D.J. Donaldson (University of Toronto).
Laser Spectroscopy of Predissociating Molecules.
- 3) F. Bouchard, J.W. Hepburn and T.B. McMahon (University of Waterloo).
Clustering Reactions and Thermochemistry of Laser Ablated Metal Ions.
- 4) M.P. Banjavcic, T.A. Daniels, R.P. Hammond and K.T. Leung (University of Waterloo).
Valence-Shell Electronic Structure of Cyclopropane by Symmetric Noncoplanar ($e,2e$) Spectroscopy.
- 5) B.W. Callen, K. Griffiths, U. Memmert, D.A. Harrington, S.J. Bushby and P.R. Norton (University of Western Ontario).
The Adsorption of Water on Ni(110): Monolayer, Bilayer, and Related Phenomena.
- 6) B.I. Niefer, P.J. Kuntz and J.J. Sloan (University of Waterloo).
Multisurface Trajectory Study of the Reaction $O(^1D_2) + H_2 \rightarrow OH(X^2\Pi;v) + H$.
- 7) F. Markel and Anne B. Myers (University of Rochester).
Resonance Raman Spectroscopy of Photodissociating Methyl Iodide in Hexane.
- 8) T.D. Pope, S.J. Bushby, B.W. Callen, K. Griffiths, C.-S. Zhang and P.R. Norton (University of Western Ontario).
Interaction of Oxygen with Clean Ni(100) and its Oxides.
- 9) S.J. Bushby, K. Griffiths, U. Memmert, D.K. Creber, R.S. Timsit and P.R. Norton (University of Western Ontario).
Adsorption of Water on Al(100).
- 10) C. Li and T.B. McMahon (University of Waterloo).
Determination of Stabilities and Structures of Cluster Ions $Cl^-(RH)$ (Cl^- attached with Alkanes).
- 11) M. Thachuk and F.R. McCourt (University of Waterloo).
Corrected Coupled States Calculations of Some Effective Cross Sections for H_2 He.
- 12) J.J. Sloan, B.I. Niefer and E.J. Kruus (University of Waterloo).
Experimental Product Energy Distributions in Elementary Reactions by Time-Resolved Fourier Transform Spectroscopy.

- 13) R. Wong, E.J. Weckman and J.W. Hepburn (University of Waterloo).
Laser Induced Fluorescence (LIF) Diagnostics of the OH Radical in Atmospheric Pressure Flames.
- 14) J.N. Beauregard and H.R. Mayne (University of New Hampshire).
Scattering of Van der Waals Molecules from Crystal Surfaces - An Extension of the Binary Collision Model.
- 15) T.L. Haslett, L.M. Cousins and M. Moskovits (University of Toronto).
Generation of Mass Selected Metal Clusters for Spectroscopic Studies in Rare Gas Matrices.
- 16) L.M. Cousins, R.J. Levis and S.R. Leone (JILA and NIST, University of Colorado).
Translationally Hot, Rotationally Cold NO Molecules from the 193 nm Explosive Vaporization of NO Films.
- 17) S.P. Sapers, V. Vaida and R. Naaman (University of Toronto).
MPI Study of Methyl Iodide in Clusters.
- 18) D.S. Green (University of Toronto).
Vibrational State Mixing in Excited Electronic States of Xe₂.
- 19) E. Ou, S. Roy, R.J. Puddephatt and P.R. Norton (University of Western Ontario).
MOCVD of Platinum: *In situ* Characterization of Decomposition Process Using FTIR.
- 20) D. Chartrand and R.J. Le Roy (University of Waterloo).
Pulling, Packing and Stacking of Rare-Gas SF₆ Clusters.
- 21) J.A. Jackman, L. Dignard-Bailey, R.S. Storey, C. MacPherson, S. Rolfe, L. van der Zwan and T.E. Jackman (NRC, Ottawa).
Matrix Effects in Secondary Ion Mass Spectrometry (SIMS) Depth Profiles of SiGe Superlattices.
- 22) R. Böhling, A.C. Becker, K. Seranski and U. Schurath (Universität Bonn/FRG and University of Toronto).
Excitation of O₂(a¹Δ_g, b¹Σ_g⁺) and I(²P_{1/2}) by Energy Transfer from I₂ (A, A', 3Π_{1,2n}) in Solid Rare Gases.
- 23) J.J. Fisher and T.B. McMahon (University of Waterloo).
Determination of Radiative Association Rate Constants by Fourier Transform Ion Cyclotron Resonance Spectroscopy.
- 24) J.W. Hepburn, W. Kong and C. Starrs (University of Waterloo).
Nonlinear Photofragmentation Spectroscopy of CS₂.
- 25) L.M. Hitchcock, G.-S. Kim, E.W. Rothe and G.P. Reck (Wayne State University).
State Selective Population Analysis of H₂(v" = 1, J" = 1) Using a Single Tunable ArF Excimer Laser.
- 26) G.-S. Kim, L.M. Hitchcock, E.W. Rothe and G.P. Reck (Wayne State University).
State Selective Detection of O₂ Via Predissociative LIF.
- 27) J. Wright and I. Hamilton (University of Ottawa and Carleton University).
Potential Energy Surface for Large Amplitude Motion and Vibrational Spacings for FH₂⁺.
- 28) V.J. Barclay and J. Wright (Carleton University).
MRD-CI Potential Surfaces Using Balanced Basis Sets: Correlation of Bond Order with Bond Function Composition.

SESSION V: Sunday, November 5, 1989

Davis Centre 1302

Chairman: J.W. Hepburn

- 9:30 - 10:10 R. Lipson (University of Western Ontario)
VUV Laser Spectroscopy of Reactive States: Valence to Ion-Pair Transitions of Halogens.
- 10:10 - 10:30 P. Hackett, H. Niki and B. Simard, (NRC, Ottawa)
High Resolution Spectroscopy of Diatomic Molecules Containing a Transition Element: The Dipole Moment and Nuclear Hyperfine Structure of TiN and its Ground $X^2\Sigma^+$ and Excited $A^2\Pi$ Electronic States.
- 10:30 - 10:50 **Coffee Break**
- 10:50 - 11:30 V.H. Smith (Queen's University)
Adventures in the 3-Body Problem: Exotic Molecules.
- 11:30 - 11:50 C. Brown, C. Callender, H. Niki, S. Mitchell, B. Simard, D. Rayner and P. Hackett (NRC, Ottawa).
Sticking to Metal Atoms: The Influence of SO Coupling on VdW Bonding Down Group XIII, and Measurements of the Strength of Agostic Bonds to Group VI Centre Using TRIR Spectroscopy.
- 11:50 - 12:10 T. Slee (University of Waterloo), D.M.P. Mingos and L. Zhenyang (Univ. of Oxford)
Bonding Models for Metal and Non-Metal Clusters.
- 12:10 - 12:30 D.M. Wardlaw and W. Jaworski (Queen's University).
Chaos in Quantum Scattering.